# Screening for Candidate Pesticides

- **Concepts**
  - Cumulative multipathway exposures
  - Intake fraction
  - Chemical properties and fate
- **Modeling approach**
- **Three examples**
  - Glyphosate
  - Octhilinone
  - Fipronil

Energy use
Industry
Agriculture
Buildings
Transportation
Consumer products

Sources & emissions

air
plants
water
soil layers
sediment

Air
Air (moving phase)
Soil tracking
Non-moving phases (floor, carpet, walls, dust, surface films)
Cleaning
Reactions

Personal air

Exposure events

Disease

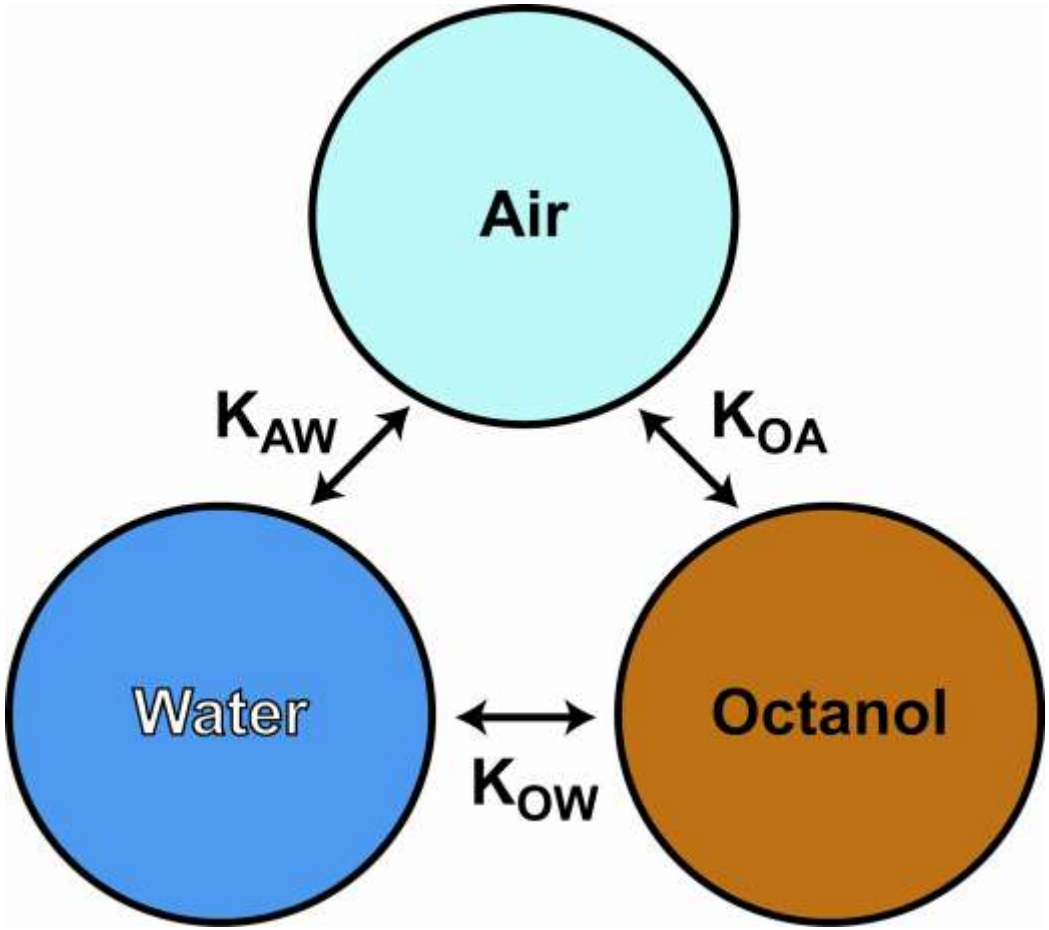
saliva
lung
skin
fat
muscle
liver

Biokinetics & toxicology

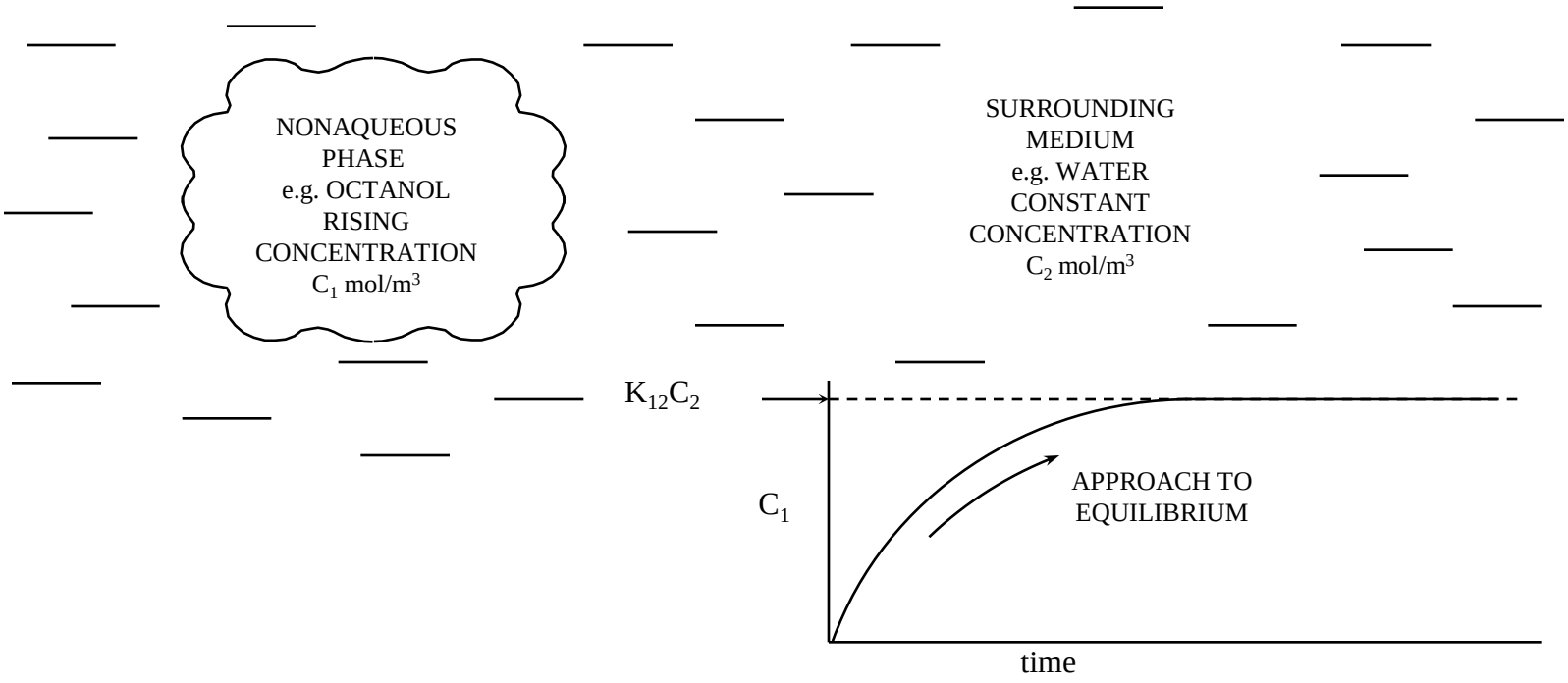
nasal
oral
dermal

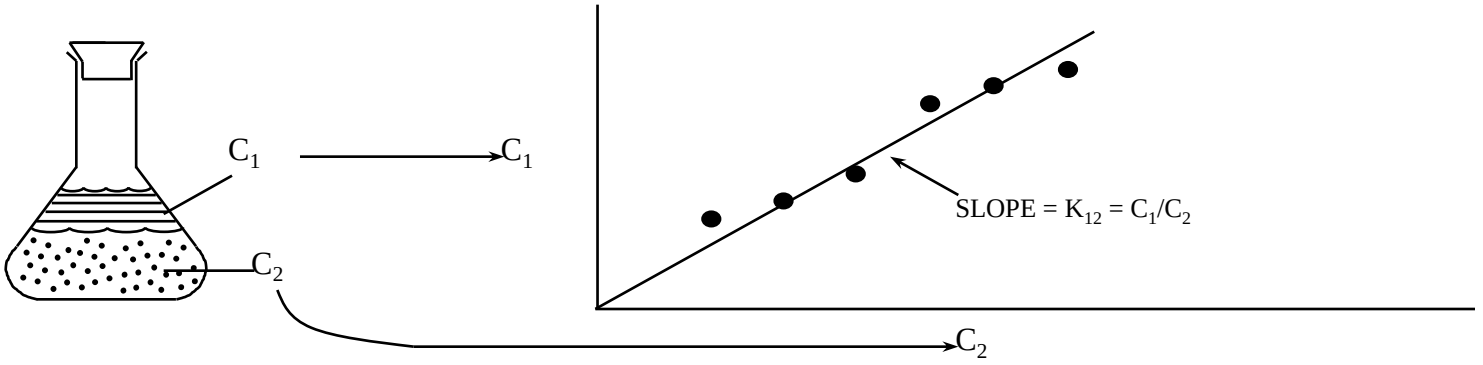
Intake and uptake

# The long-term behavior chemicals in the environment is determined by their partitioning between 3 available media:

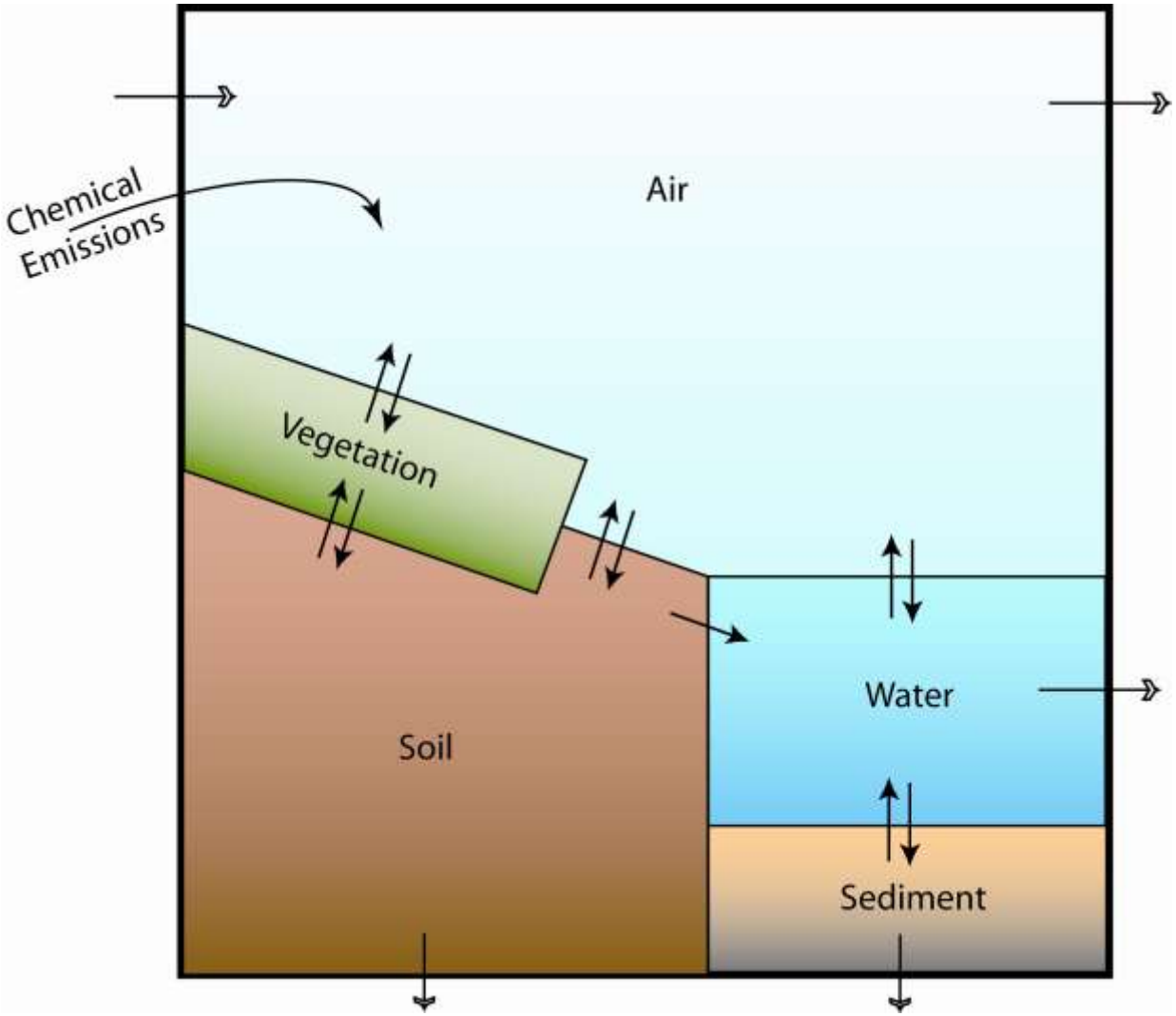


# Experimental Determination of Partition Coefficients

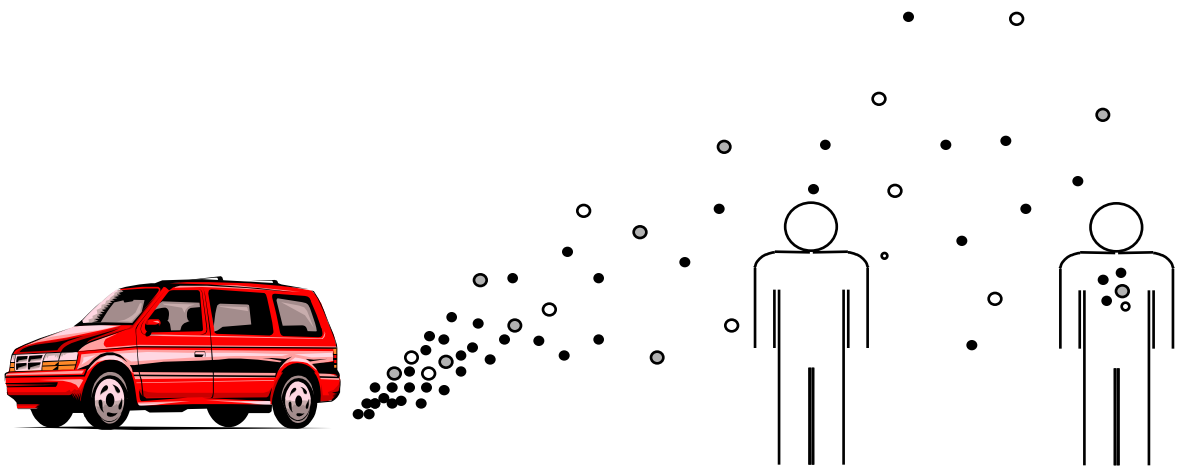


# Level III multimedia contaminant fate model



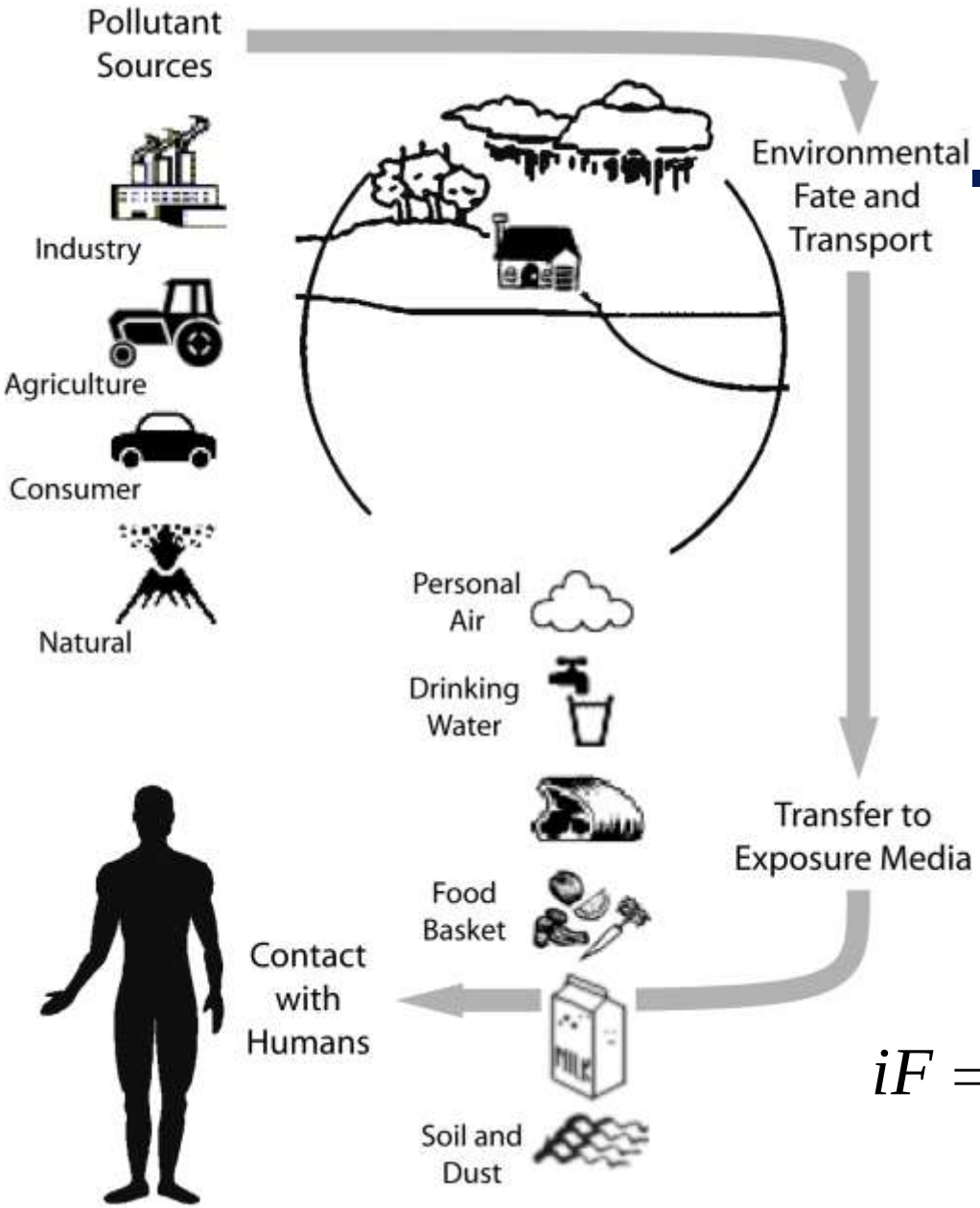
# Intake fraction (iF) Concept

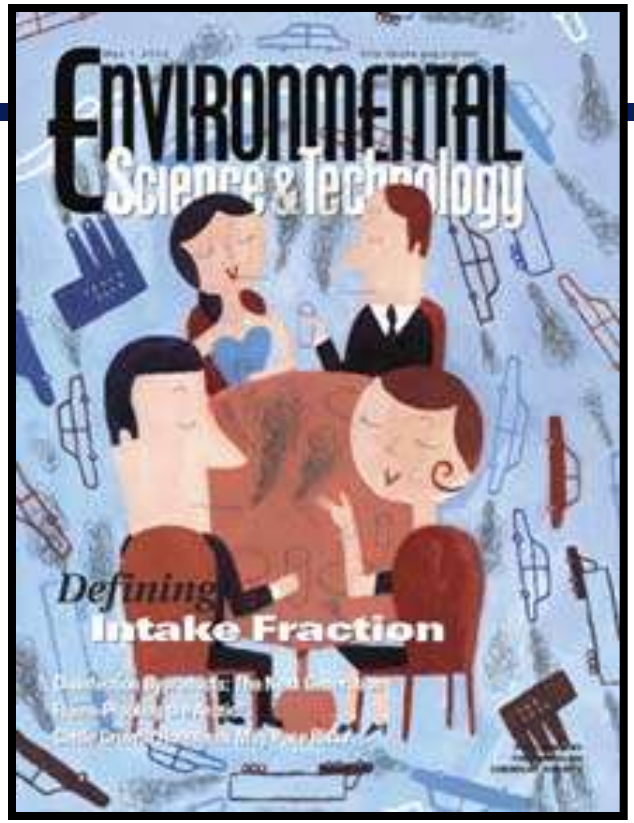


emissions → concentration → exposure → intake

emissions ⟶ intake

$$\text{Intake Fraction} = \frac{\text{mass inhaled}}{\text{mass emitted}}$$

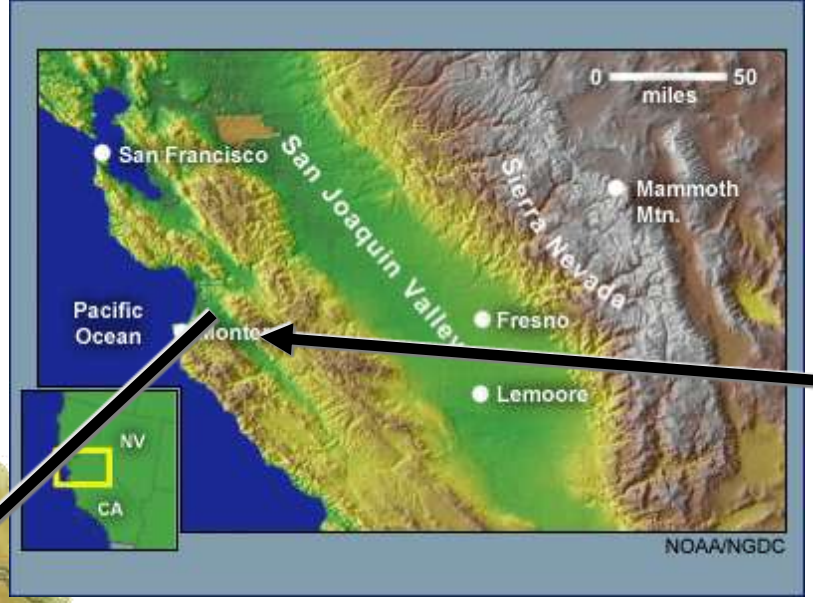


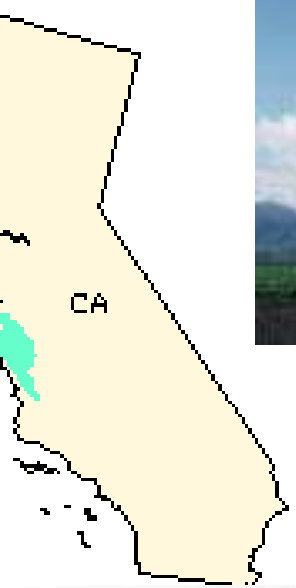




$$iF = \frac{Population\,Intake\,(mg/day)}{Emission\,Rate\,(mg/day)}$$

# Factors that Influence iF

- **Proximity:**
  **location of people (or their food and water) relative to source**
- **Persistence:**
  **pollutant transport & transformation**
- **Mobility:**
  **temporal & spatial variations**
  - **pollutant concentration**
  - **population activities**



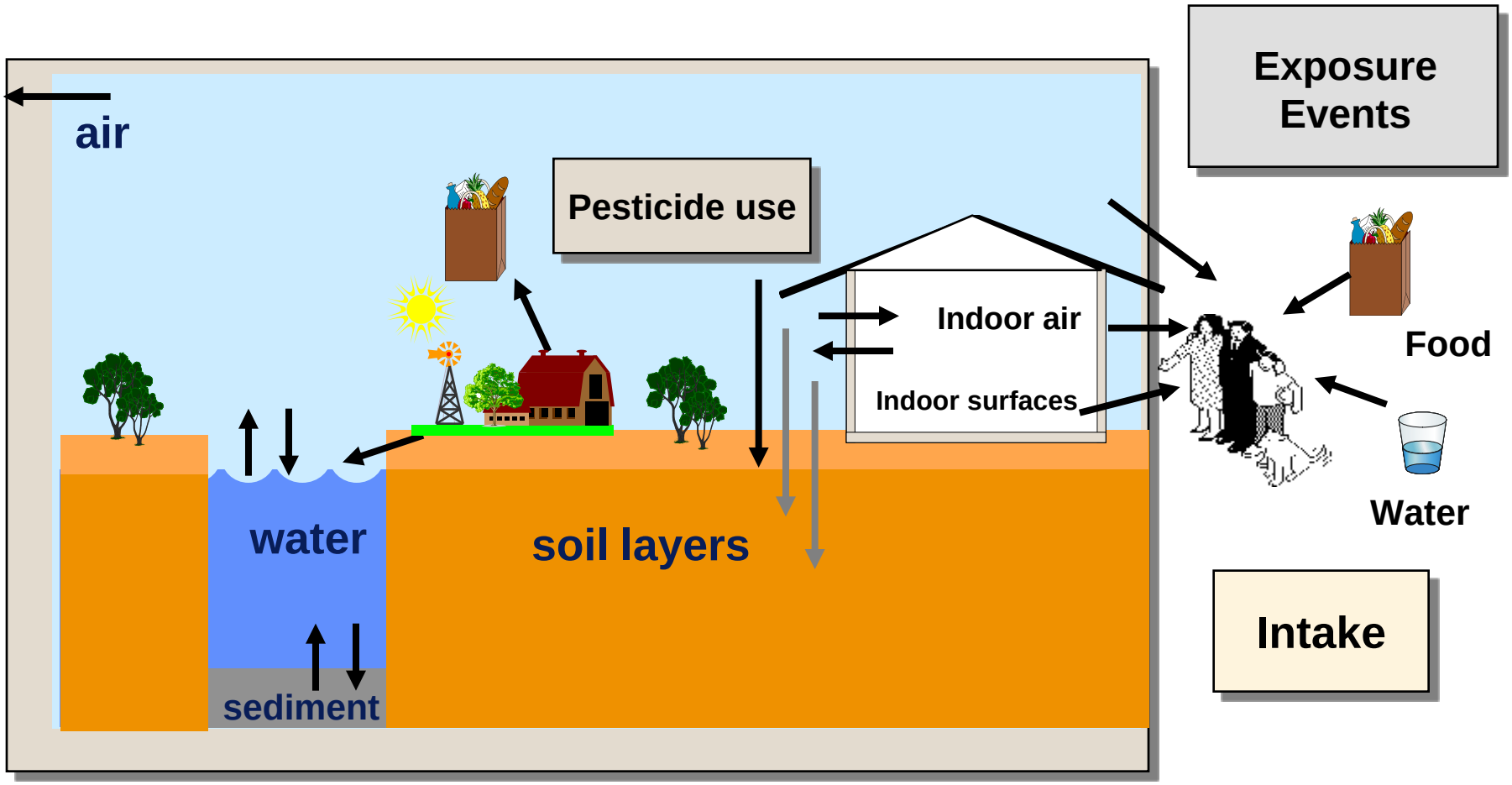





CHAMACOS

CENTER FOR THE HEALTH ASSESSMENT OF MOTHERS AND CHILDREN OF SALINAS

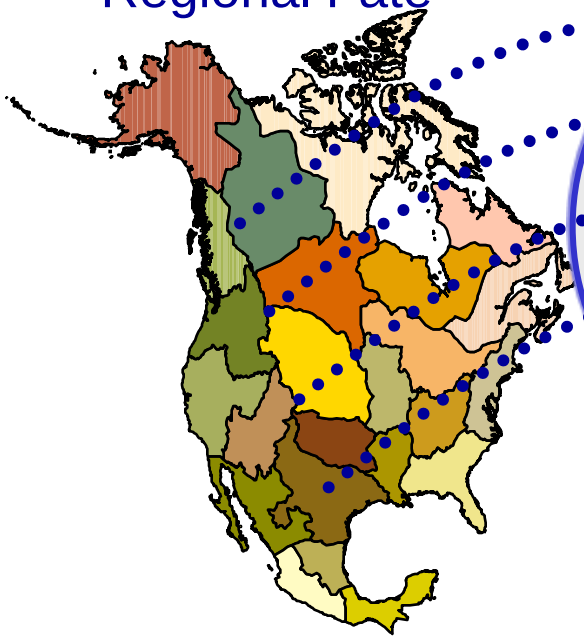
# CalTOX Model Schematic



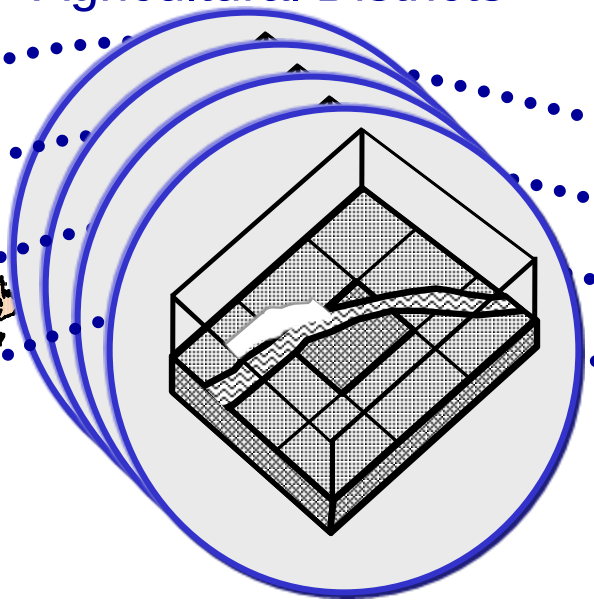

**Environmental transport and transformation (outdoors, indoors, and to food)**

# Dietary Exposures

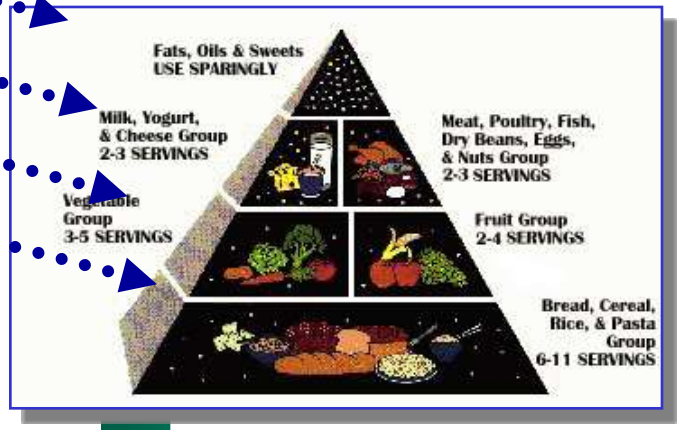
Regional Fate



Agricultural Districts



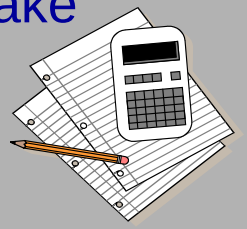
Food Supply
(Regional or Local)




Chemical Residue Data

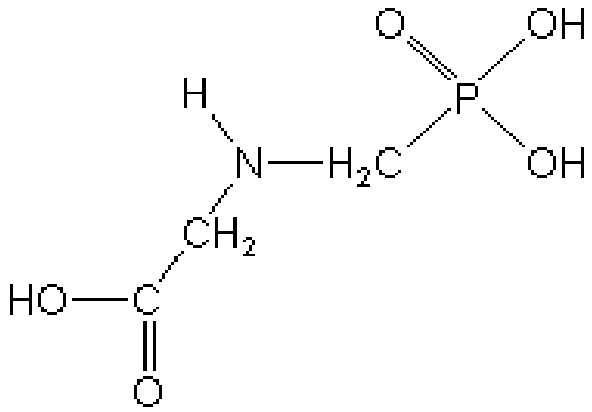
Recipe Files

Food Intake Survey Data



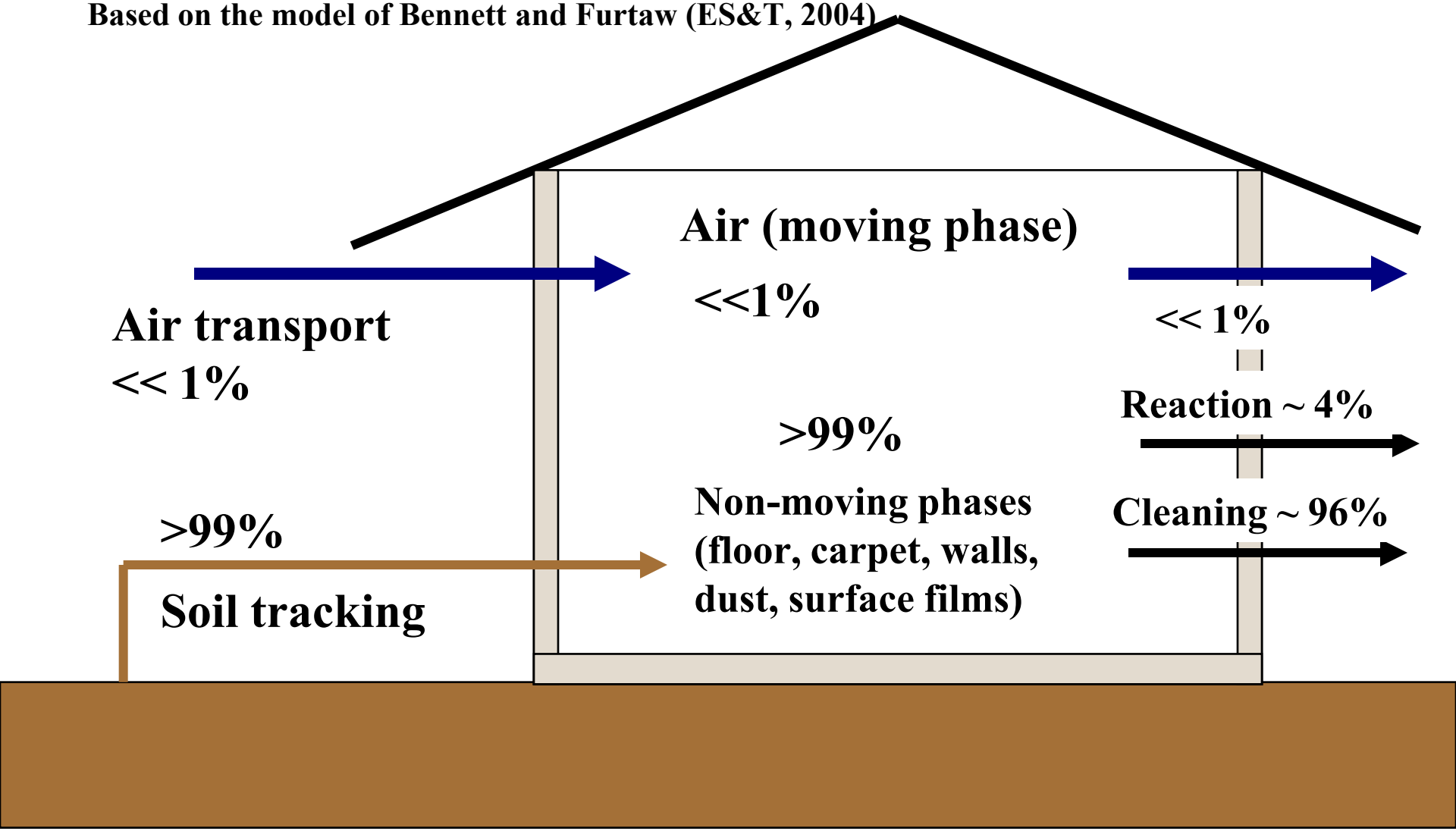
Cohort

# Glyphosate

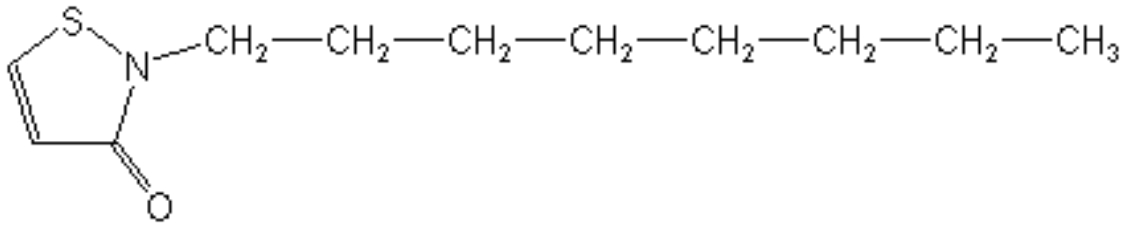



- **MW: 169.07**
  **Log Kow: -4**
  **Log Kaw: -12.65**
- **Very water soluble, very low vapor pressure, binds strongly to soil (Koc is ~3000)**
- **Environmental distribution: primarily retained in upper soil layers**
- **Regional iFi (individual intake fraction): 5.2 E-10 (high)**
- **Dominant human exposure: exposed produce (assuming 1 to 5% home/local sources)**
- **Indoor iFi: 0.013 (very high)**

# Indoor Mass Balance
## (Glyphosate)



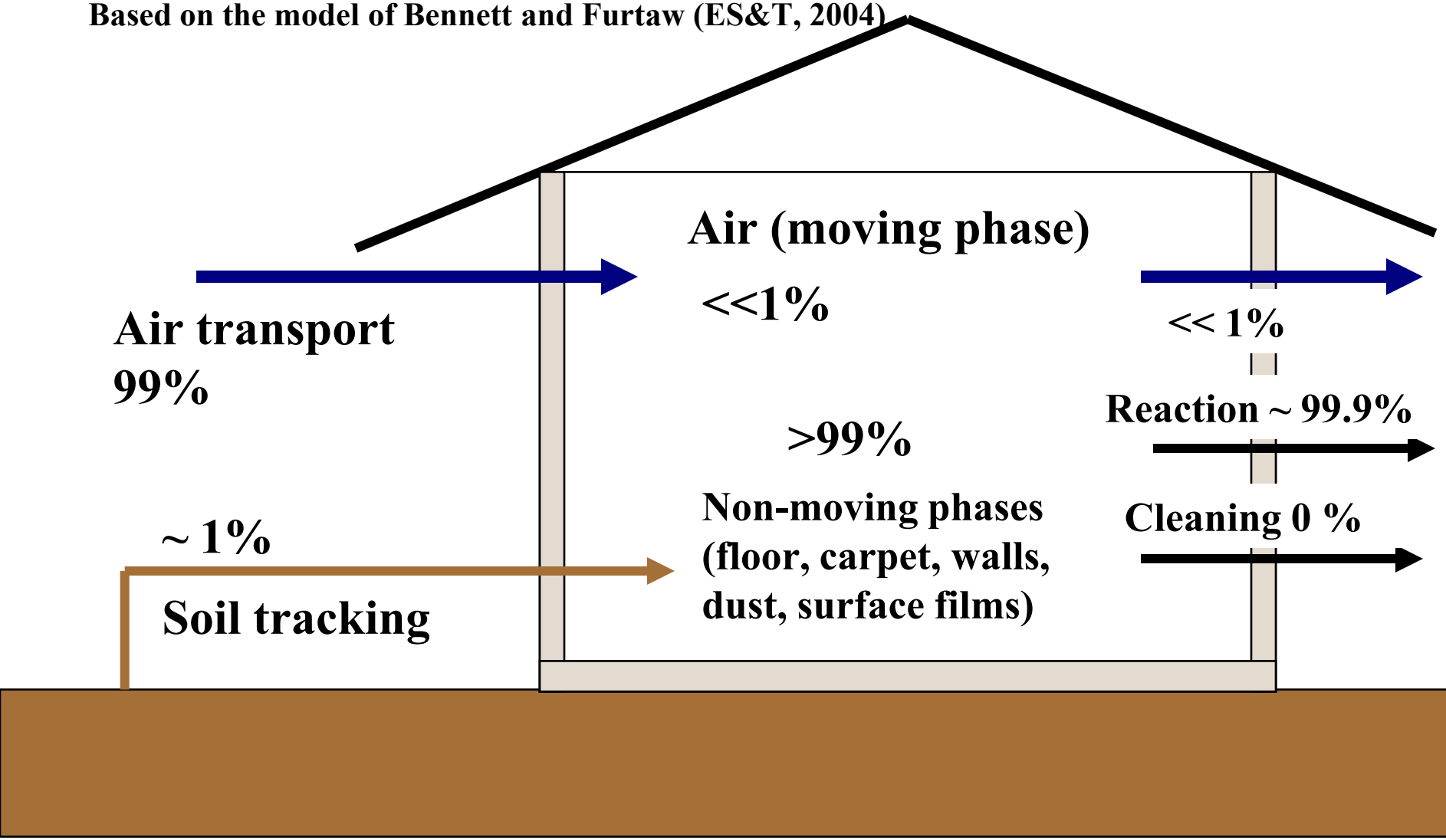
# Octhilinone



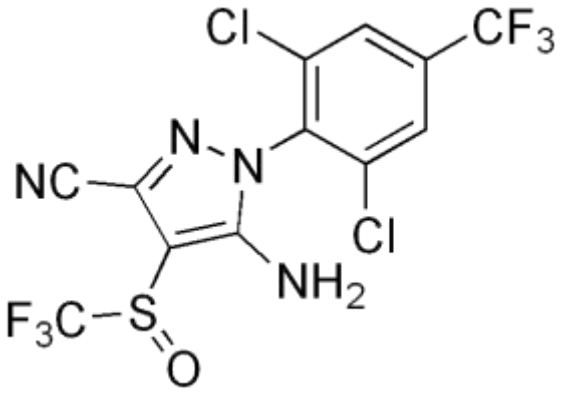

- **MW: 213.34**
  **Log Kow: 2.45**
  **Log Kaw: -2.68**
- **Partitions to water and lipids; semi-volatile**
- **Environmental distribution: primarily retained in upper soil layers and surface water**
- **Regional iFi (individual intake fraction): 2.5 E-11**
- **Dominant human exposures: drinking water and then indoor pathways**
- **Indoor iFi: 8 E-6**

# Indoor Mass Balance
## (Octhilinone)

Based on the model of Bennett and Furtaw (ES&T, 2004)



# Fipronil




- **MW: 213.34**
  **Log Kow: 4.00**
  **Log Kaw: -4.07**
- **Partitions to carbon and lipids; low volatility**
- **Environmental distribution: primarily retained in upper soil layers**
- **Regional iFi (individual intake fraction): 5.8 E-11**
- **Dominant human exposures: local/homegrown food and then indoor pathways**
- **Indoor iFi: 2.5 E-5**

# Indoor Mass Balance
## (Fipronil)

Based on the model of Bennett and Furtaw (ES&T, 2004)